

# **FALL 2011 FINAL PROJECT**

Student 2

THE COOPER UNION FOR THE ADVANCEMENT OF SCIENCE AND ART

ChE142: Mass Transfer and Separation Process Principles

Professor B. Davis

Fall 2011

Date of Submission: Monday, December 12, 2011

## MEMO

**To:** Benjamin Davis, Project Manager, C Squared Consulting Associates, 41 Cooper Square, NY, NY 10003

**From:** Student 2, Design Engineer, C Squared Consulting Associates, 41 Cooper Square, NY, NY 10003

**Subject:** Initial Proposal for Separation of a Four Component Mixture

**Date:** Monday, December 12, 2011

This is a memo regarding an initial proposal for a separation plant to separate a 1000 kg mixture of ethylbenzene (90%), ethanol (8%), ammonia (1%) and hydrogen sulfide (1%). Thermodynamic data was based on the Peng-Robinson model (including data to calculate minimum work). Separation units were sized and costed. Sizing was done using Pro/II and confirmed by graphical and analytical methods. Costing was based on Analysis, Synthesis, and Design of Chemical Processes, by Turton *et al.*, 2nd edition.

This initial design is comprised of four distillation columns and a membrane. It separates the mixture to four streams with at least 99% purity by mole while expending less than ten times the minimum work required to perform such a separation. The sizes of these columns are quite small where diameters range from 0.2 to 1 ft and heights range from 10 to 24 ft. It is probable that these columns cannot physically be built and stand. Based on Turton *et al.*, the linear velocity was assumed to be 2 ft/sec. The extremely small diameters of two of the columns (Column 2 and Column 3 in the PFD, See Appendix I) were calculated because diameter sizing is based on vapor flow rates. Vapor flow rates depend on the amount of light key components in the column. Ammonia and ethanol in columns 2 and 3, respectively, are quite low in comparison to the amount of heavy key present (ethylbenzene and ethanol respectively). Consequently, the cost of the column shells and trays are low as well, totaling about \$29,000. Reboilers and condensers were sized to have areas ranging from  $1.4 \times 10^{-4}$  to  $5.4 \times 10^{-2}$  m<sup>2</sup> and costing was based on prices for kettle reboilers and double pipe condensers. Costing for these heat exchangers were overestimated because costing information was only valid for equipment larger than those specified in this PFD. Total costs for heat exchangers came to \$33,000.

The thermoplastic polyphenylene sulfide membrane that is used to further separate a mixture largely composed of ammonia and hydrogen sulfide has an area of  $1.5 \times 10^6$  ft<sup>2</sup> and a thickness of 0.00085 mil. The pressure of the feed entering the membrane is 29 psia and the pressure on the permeate side of the membrane is 2 psia. Professional Plastics ([www.professionalplastics.com](http://www.professionalplastics.com)) was used to cost the polyphenylene sulfide film used for the membrane. DIPPR was used to determine permeance for this material. Cost per membrane was roughly \$22,000.

Taking into account the utilities that are needed for the condensers and reboilers, and annual membrane replacements for a ten-year plant life, capital costs and annual costs for that time period total to about \$300,000. This is relatively cheap for a plant but the lack of feasibility for building such a plant due to the size of the columns suggests that further examination of the process is necessary. Safety issues should be explored if such pressure conditions are considered when building a membrane.

See appendices for a PFD of this design and other related details. Let me know if you have any questions and I will keep you posted on future work.

## Appendices

### Appendix I - Process Flow Diagram

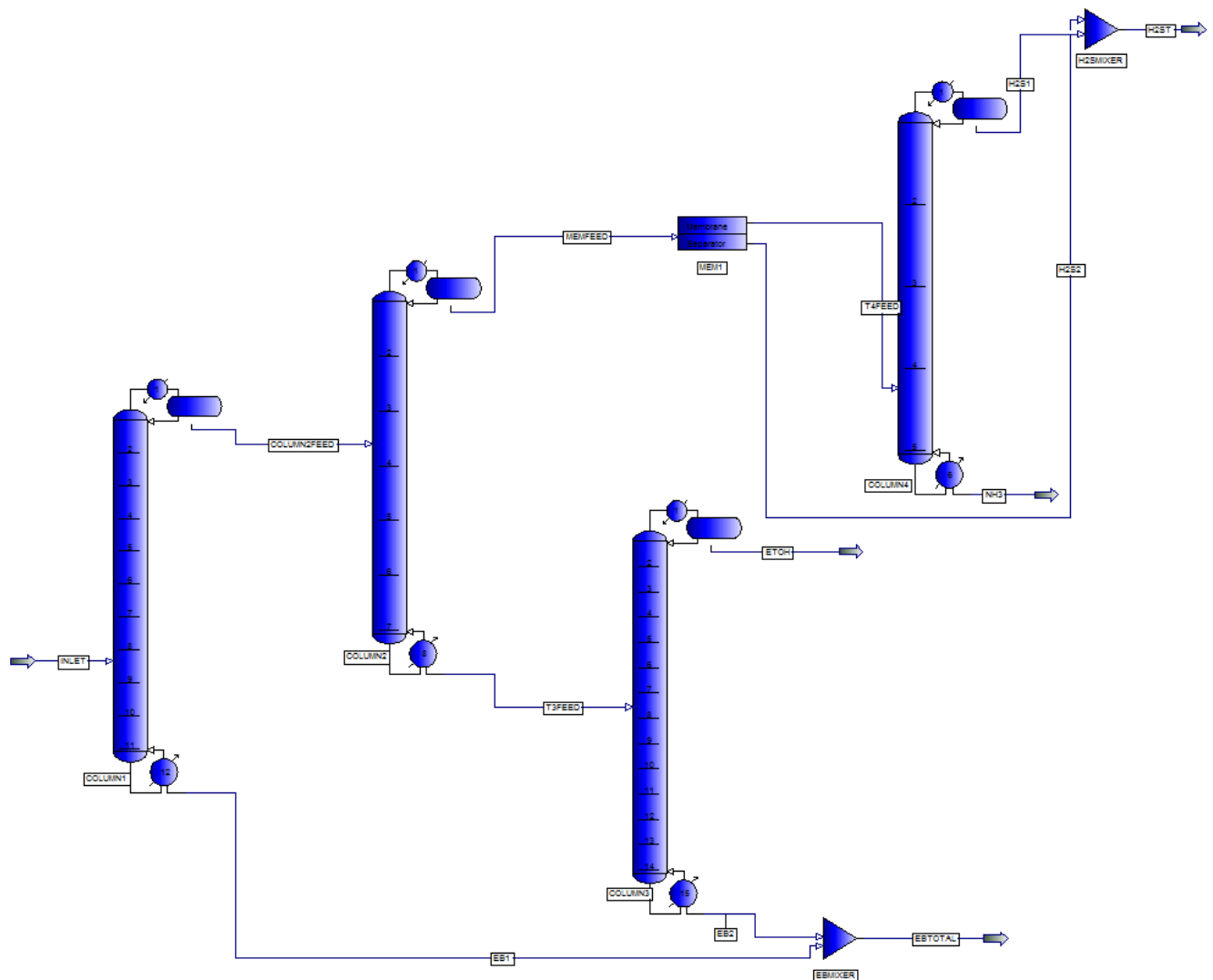


Figure 1: Process flow diagram of initial proposal for separation of ethylbenzene (90%), ethanol (8%), ammonia (1%), & hydrogen sulfide (1%).

**Appendix I (cont'd)**

In order to understand qualitatively and quantitatively how the mixture is being separated in the PFD, note that ethylbenzene is abbreviated as EB, ethanol as ETOH, ammonia as NH<sub>3</sub>, and hydrogen sulfide as H<sub>2</sub>S. See tables below for more details.

PFD Label Name	Description of Equipment/Feed
FEED	Contains EB (90%), ETOH (8%), NH <sub>3</sub> (1%), and H <sub>2</sub> S (1%), 1000 kg/hr
COLUMN1	Separates out EB, Light Key (LK): ETOH, Heavy Key (HK): EB
EB1	Stream of 99.8% EB by mole; To be mixed with EB2 to give EB product stream
COLUMN2FEED	Contains mostly ETOH, NH <sub>3</sub> , H <sub>2</sub> S
COLUMN2	Separates ETOH from NH <sub>3</sub> and H <sub>2</sub> S (LK: NH <sub>3</sub> , HK: ETOH)
COLUMN3FEED	Contains mostly ETOH
COLUMN3	Separates ETOH from EB (LK: ETOH, HK: EB)
EB2	Stream of 100% EB; To be mixed with EB1 to give EB product stream
MIXER1	Mixes EB1 & EB2 to give EB product stream
EBT	EB product stream, 99.8% EB by mole, 8.47 kmol/hr
ETOH	Ethanol product stream, 98.5% ETOH by mole, 1.745 kmol/hr
MEMFEED	Contains mostly NH <sub>3</sub> and H <sub>2</sub> S
MEM1	Separates NH <sub>3</sub> & H <sub>2</sub> S
COLUMN4FEED	Permeate of membrane, Contains mostly NH <sub>3</sub> and some H <sub>2</sub> S
H2S2	Retentate of membrane, Contains mostly H <sub>2</sub> S
COLUMN4	Separates NH <sub>3</sub> and H <sub>2</sub> S
NH3	NH <sub>3</sub> product stream, 99% NH <sub>3</sub> by mole, 0.589 kmol/hr
H2S1	Stream of 99% H <sub>2</sub> S by mole; To be mixed with H <sub>2</sub> S2 to give H <sub>2</sub> S product stream
MIXER2	Mixes H <sub>2</sub> S1 & H <sub>2</sub> S2 to give H <sub>2</sub> S product stream
H2ST	H <sub>2</sub> S product stream, 99.1% H <sub>2</sub> S by mole, 0.290 kmol/hr

Table 1: **Description of PFD labels.**

Component/Parameter	FEED	Stream											
		COLUMN2FEED	EB1	MEMFEED	COLUMN3FEED	ETOH	EB2	COLUMN4FEED	H2S2	H2S1	NH3	EBT	H2ST
Phase	Mixed	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Vapor	Mixed	Liquid	Liquid	Mixed	Mixed
Temperature (F)	170.3	35.6	338.3	-26.1	223.4	213.6	350.5	-26.1	-26.1	-145.0	-97.5	338.3	-144.4
Pressure (psia)	29.4	29.0	34.0	29.0	34.0	34.0	39.0	2.0	29.0	1.5	1.5	34.0	1.5
Ethylbenzene	0.764	0.160	0.998	0	0.223	0.014	1.000	0	0	0	0	0.998	0
Ammonia	0.053	0.190	0	0.665	0.001	0.001	0	0.880	0.004	0.010	0.990	0	0.006
Hydrogen sulfide	0.026	0.095	0	0.334	0	0	0	0.120	0.991	0.990	0.010	0	0.991
Ethanol	0.157	0.556	0.002	0.001	0.776	0.985	0	0	0.004	0	0	0.002	0.003
Molar Flowrate (kg <sub>mol</sub> /hr)	11.094	3.094	8.000	0.879	2.215	1.745	0.470	0.664	0.215	0.075	0.589	8.470	0.290

Table 2: Composition and molar flow rates of all streams.

**Appendix II - Mass Recovered**

To confirm that no more than 90% of the original feed's mass was lost to waste or burned for heat, the mass recovered was determined by summing the mass flow rates of the product streams and comparing it to the mass flow rate of the feed.

Product Stream	Molar Flow Rate (kmol/hr)
EB	8.47
ETOH	1.75
NH3	0.59
H2S	0.29
Total	11.1

Table 3: **Molar flow rates of outlet/product streams.**

The inlet feed's molar flow rate was 11.1 kmol/hr. The percent of mass recovered:

$$\frac{\text{Mass Flow Rate In}}{\text{Mass Flow Rate Out}} = \frac{11.1}{11.1} \times 100\% = 100\% \quad (1)$$

This confirms that no mass was lost due to waste streams or burned for heat. This fulfills the requirement that no more than 90% of the mass should be wasted.

### Appendix III - Calculation and Comparison to Minimum Work Required

The minimum work of separation is defined as (Separation Process Principles, by Seader *et al.*:

$$W_{min} = \Sigma_{out} nb - \Sigma_{in} nb \quad (2)$$

where

$$b = h - T_0 s \quad (3)$$

and  $T_0$  = ambient temperature

There was one stream into the system (FEED) and four streams coming out of the system (EB, ETOH, NH<sub>3</sub>, H<sub>2</sub>S). For each stream,  $nb$  was calculated:

$$nb = \dot{m} \times (h - T_0 s) \quad (4)$$

where  $\dot{m}$  = mass flow rate (kg/hr),  $h$  = specific enthalpy (BTU/kg),  $T_0$  = ambient temperature (F),  $s$  = specific entropy (BTU/kgF)

For FEED:

$$1000 \text{ kg/hr}(150.03 \text{ BTU/kg} - (300 \text{ F} * 2.54 \text{ BTU/kgF})) = -610993 \text{ BTU/hr} \quad (5)$$

For EBT:

$$898.18 \text{ kg/hr}(310.14 \text{ BTU/kg} - (300 \text{ F} * 2.71 \text{ BTU/kgF})) = -450387 \text{ BTU/hr} \quad (6)$$

For ETOH:

$$81.82 \text{ kg/hr}(254.11 \text{ BTU/kg} - (300 \text{ F} * 2.74 \text{ BTU/kgF})) = -46450 \text{ BTU/hr} \quad (7)$$

For NH<sub>3</sub>:

$$10.13 \text{ kg/hr}(-281.15 \text{ BTU/kg} - (300 \text{ F} * 2.81 \text{ BTU/kgF})) = -11392 \text{ BTU/hr} \quad (8)$$

For H<sub>2</sub>S:

$$9.88 \text{ kg/hr}(30.53 \text{ BTU/kg} - (300 \text{ F} * 2.19 \text{ BTU/kgF})) = -6181 \text{ BTU/hr} \quad (9)$$

Calculating  $W_{min}$ ,

$$W_{min} = (-450387 + -46450 + -11392 + -6181) - (-610993) = 96693 \text{ BTU/hr} \quad (10)$$

The maximum  $W$  allowed is ten times  $W_{min}$  which is 966934 BTU/hr.

To determine the work used in this PFD, the heat duties of all of the reboilers and condensers were considered: Heat duties of reboilers were contributed to the work used and those of the condensers released work that could be used elsewhere.

**Appendix III - Calculation and Comparison to Minimum Work Required (cont'd)**

Equipment	Heat Duty (BTU/hr)
Column 1, Condenser	-258500
Column 1, Reboiler	371400
Column 2, Condenser	-19300
Column 2, Reboiler	50400
Column 3, Condenser	-86800
Column 3, Reboiler	90600
Column 4, Condenser	-31600
Column 4, Reboiler	12800

Table 4: **Work used/released by column condensers and reboilers.**

Based on the values in Table 15, work used in this PFD was calculated to be 129000 BTU/hr, which is well under the maximum allowable work to be used for the separation.



### Appendix IV - Number of Trays of Column from Pro/II & Graphical Confirmation of Distillation Column Sizing for Columns 1-4

Column	Number of Trays
Column 1	12
Column 2	8
Column 3	15
Column 4	6

Table 5: **Number of trays in distillation columns from Pro/II.**

For confirmation, see attached pages for these calculations done graphically via McCabe-Thiele Method. The number of trays determined graphically were of the same magnitude as those found via Pro/II (above). The McCabe-Thiele Method is outlined below:

1. Generate binary vapor liquid equilibrium data and  $x = y$  line using Pro/II. Specify the light key as the "first component"
2. Determine the concentration of the light key in the feed ( $z_f$ ), the concentration of the light key in the distillate ( $x_D$ ), and the concentration of the light key in the bottoms ( $x_B$ ).
3. Determine  $q$  based on the conditions of the feed.
4. Determine  $q$ -line equation based on its equation:

$$y = \left(\frac{q}{q-1}\right)x - \frac{z_F}{q-1} \quad (11)$$

5. Because all feeds were assumed to be liquid,  $q = 1$  and  $q$ -lines were vertical and passed through  $z_F$  on the  $x$ -axis.
6. The minimum L/V lines were drawn - the rectifying section passed through the  $x=y$  line at  $x = 0.99$  and where the  $q$ -line intersects the equilibrium curve, and the stripping section passed through where the  $q$ -line intersects the equilibrium curve and the  $x=y$  lines at  $x = 0.01$ .
7. The minimum number of trays was determined by drawing steps between the  $x=y$  line and the equilibrium curve.
8. The slope of the L/V minimum line, rectifying section, was found and set to  $\frac{R_{min}}{R_{min}+1}$ .  $R_{min}$  was calculated.
9. The following relationship from Turton et al. heuristics was used to determine  $R$ ,  $R = 1.5R_{min}$ .
10. This value of  $R$  was used to determine the slope of the actual L/V line, rectifying section.
11. The actual L/V line was plotted and steps were drawn between this line and the equilibrium curve to determine the actual number of trays.

Please note the following things about the graphs:

- One McCabe-Thiele plot was done for Columns 1, 2, 3 for initial and revised designs because similar if not the same conditions (pressure of feed, and compositions of the feed, distillate, and bottoms) occurred
- A ratio of 1.5 for  $R/R_{min}$  was used based on heuristics from Turton *et al.*. This differs from the  $R$  used in Pro/II calculations. This may contribute to discrepancies between the actual trays numbers calculated by Pro/II and graphically.
- The blue line in each plot is the  $45^\circ$  line, which represents the reflux ratio when there is infinite reflux.
- The green line in each plot represents the equilibrium data for the binary mixture.
- The composition of the light key  $z_f$  used in the plot was adjusted when assuming a pseudo-binary mixture using the following normalization:

$$z_f = \frac{\text{Mole fraction of Light Key}}{\text{Mole fraction of Light Key} + \text{Mole fraction of Heavy Key}} \quad (12)$$

- The mole fractions of the light key in the distillate and bottoms ( $x_D$  and  $x_B$  respectively) was calculated from Pro/II results and if they were greater than 0.99 or less than 0.01, respectively, values were just taken to be 0.99 or 0.01, respectively because it is difficult to graph values greater than 0.99 or less than 0.01.
- It was assumed that all feeds were at its bubble point so all the feed was a liquid. This led  $q$  to equal 1 and the  $q$ -line to always be a vertical line that passed through  $z_f$ , the composition of the light key in the feed.
- The "count" of the minimum number of trays is "inside" the step on the graph and the "count" of the actual number of trays is "outside" the step on the graph.

## Appendix V - Diameter Sizing for Columns 1-4

Below is a sample calculation for how the height and diameter was sized for Column 1. See attached page for heights and diameters of Columns 2 - 4.

For column 1:

### Height of a Distillation Column

Based on heuristics from Turton *et al.* (Chapter 9, Table 9.13 and 9.14), tray spacings were assumed to be 20 inches. Heuristics also give heights for top spacing for vapor disengagement and bottom spacing for liquid level and reboiler return based on a 3 ft in diameter column. Based on a 3 ft diameter, top spacing was 4 ft and bottom spacing was 6 ft. Space at the top and bottom were calculated in proportion to the diameter of the designed columns but a maximum of 20 ft for both the top and bottom spacings were added. For column 1, the top spacing was calculated to be 1.31 ft and the bottom spacing was calculated to be 1.97 ft.

To determine the height of the column:

$$(\text{Number of Trays} - 1) \times (\text{Tray Spacing}) + \text{Top Spacing} + \text{Bottom Spacing} = \text{Height} \quad (13)$$

$$(12 - 1) \times (20 \text{ in.}) + 1.31 \text{ ft} + 1.97 \text{ ft} = 21 \text{ ft} \quad (14)$$

**Diameter of a Distillation Column** The maximum vapor flow rate was determined by to 167 m<sup>3</sup>/hr (1.64 ft<sup>3</sup>/sec) from the Pro/II report. Based on heuristics from Turton *et al.*, the linear velocity of the vapor was assumed to be 2 ft/sec.

To determine the area of the tray needed for this vapor flow rate to pass at that specified velocity,

$$\frac{\text{Vapor flow rate}}{\text{Linear velocity}} = \text{Area} \quad (15)$$

$$\frac{1.64 \text{ ft}^3/\text{sec}}{2 \text{ ft/sec}} = 0.82 \text{ ft}^2 \quad (16)$$

$$\text{Diameter} = 2 \times \left( \sqrt{\frac{\text{Area}}{\pi}} \right) \quad (17)$$

$$\text{Diameter} = 2 \left( \sqrt{0.82/\pi} \right) = 1.02 \text{ ft} \quad (18)$$

Using these methods of calculation for heights and diameters of columns:

Column	Height (ft)	Diameter (ft)
Column 1	21.3	1.02
Column 2	12.14	0.18
Column 3	23.85	0.27
Column 4	10.47	0.69

Table 6: Distillation column sizing based on Pro/II and heuristics.

### Appendix VI - Membrane Sizing Calculation

Membrane size can be confirmed by finding the volumetric flow through the membrane and ensuring that the area used is appropriate. Values for permeabilities were found from DIPPR and unit conversions were done to find the values for permeance below. From values used in Pro/II:

- Thickness = 0.00085 mil
- Permeance for NH<sub>3</sub> = 0.00254 (ft<sup>3</sup>/ft<sup>2</sup>hr\*psia)
- Permeance for H<sub>2</sub>S = 0.000508 (ft<sup>3</sup>/ft<sup>2</sup>hr\*psia)
- Area = 150 ft<sup>2</sup>

Example: For ammonia:

- Total pressure of membrane feed = 29 psia
- Mole fraction of ammonia = 0.665
- Partial pressure of ammonia in feed = 19.285 psia
- Total pressure of permeate = 2 psia
- Mole fraction of ammonia = 0.749
- Partial pressure of ammonia in permeate = 1.498 psia

$$\text{Flux} = N_{\text{NH}_3} = (0.000508)(19.285 - 1.498) = 1.4\text{ft}^3/\text{ft}^2\text{hr} \quad (19)$$

The flow rate of ammonia can be found by dividing the mass flow rate of the permeate by the density of the permeate:

$$\dot{n}_{\text{NH}_3} = 19.953\text{kg/hr}/0.157\text{kg/m}^3 = 127.08\text{m}^3/\text{hr} \quad (20)$$

Dividing the flux by the flow rate will give an area for the membrane:

$$N_{\text{NH}_3}/\dot{n}_{\text{NH}_3} = \text{Area} = 0.011\text{m}^2 \quad (21)$$

Note: Not sure why this calculation is not agreeing with area used in Pro/II. I will investigate further if a membrane is used in the revised PFD.

## Appendix VII - Capital Costing (Columns and Membrane)

Using cost equations for the CAPCOST Program as specified in Turton *et al.*, sizing parameters such as area and volume were used to determine costs of the shell and trays of the column. Purchased equipment costs were determined by:

$$\log(C_p^0) = K_1 + K_2 \log(A) + K_3 [\log(A)]^2 \quad (22)$$

where  $A$  is the sizing parameter,  $K_1$ ,  $K_2$ , and  $K_3$  are constants,  $C_p^0$  is the purchased equipment costs for 2001. Using the CEPCI value for 2001 of 397 and the CEPCI value for 2011 of 564.8, current prices for these columns were calculated.

CAPCOST cost equations were fitted to columns of a specified size. If a designed column was smaller than the specified size, the minimum  $A$  value was used and thus, the cost was overestimated. If a designed column was larger than the specified size, the maximum  $A$  value was used and the price was estimated assuming a linear relationship between  $A$  and price.

For column 1:

- Volume ( $\text{m}^3$ ) = 0.49
- Area ( $\text{m}^2$ ) = 0.08
- For shell costing,  $A = 0.49$
- For shell costing,  $K_1 = 3.94974$ ,  $K_2 = 0.4485$ ,  $K_3 = 0.1074$
- For tray costing,  $A = 0.08$
- For tray costing,  $K_1 = 2.9949$ ,  $K_2 = 0.4465$ ,  $K_3 = 0.3961$

Using the above values and Equation 17, costs for year 2001 were calculated to be:

- Cost of Shell in 2001: \$2337.55
- Cost of Trays in 2001: \$1364.04

Using 2011 CEPCI value of 564.8 (from *Chemical Engineering, April 2011*) and 2001 CEPCI value of 397,

- Cost of Shell in 2011: \$3325.56
- Cost of Trays in 2011: \$4689.60

Using the above method, the following costs were calculated for Columns 2-4:

Note that because these columns were on the small size, the minimum  $A$  specified in the heuristics were used for Columns 2-4 and because of this, costing is overestimated.

See detailed calculations in last appendix for membrane costing figures. The cost of a membrane of the same material in pre-cut sizes was found at Professional Plastics. Using the density of PPS, the cost per unit mass was determined. The mass needed for the membrane in this PFD was found and through the previously calculated cost per unit mass, the price was calculated.

Column	Shell Cost (\$)	Tray Cost (\$)
Column 1	3325.56	4689.60
Column 2	2788.41	4152.45
Column 3	2788.41	4152.45
Column 4	2788.41	4152.45
Total	11690.79	17146.95

Table 7: **Distillation column costing using CAPCOST**

## Appendix VIII - Heat Exchanger Sizing & Costing

The heat duty ( $Q$ ) from Pro/II was used to determine the area of the heat exchanger needed:

$$Q = UA\Delta T_{lm} \rightarrow A = \frac{Q}{U\Delta T_{lm}} \quad (23)$$

Based on heuristics from Turton *et al.*,  $U$  was taken to be 850 W/m<sup>2</sup> and 1150 W/m<sup>2</sup> for condensers and reboilers, respectively.

For the condenser for Column 1,

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln \frac{T_1}{T_2}} \quad (24)$$

- $T_{stream,in} = 108.94$  °C
- $T_{stream,out} = 2$  °C
- $T_{utility,in} = -190.38$  °C
- $T_{utility,out} = -189.39$  °C
- $\Delta T_1 = T_{stream,in} - T_{utility,out} = 108.94 - (-189.39) = 298.32$  °C
- $\Delta T_2 = T_{stream,out} - T_{utility,in} = 2 - (-190.38) = 192.38$  °C
- $\rightarrow \Delta T_{lm} = 241.49$

$$A = \frac{71.8 \text{ J/sec}}{(850 \text{ W/m}^2)(241.49)} = 0.00035 \text{ m}^2 \quad (25)$$

Based on the CAPCOST program delineated in Turton *et al.*, the cost of heat exchangers were determined. Double pipe heat exchangers were chosen for condensers because the smallest heat exchangers do come in that type. Kettle reboilers' cost information was used for this project because kettle reboilers were chosen in the Pro/II design. The CAPCOST equation was used:

$$\log(C_p^0) = K_1 + K_2 \log(A) + K_3 [\log(A)]^2 \quad (26)$$

where  $A$  is the sizing parameter,  $K_1$ ,  $K_2$ , and  $K_3$  are constants,  $C_p^0$  is the purchased equipment costs for 2001. Again, using the CEPCI value for 2001 of 397 and the CEPCI value for 2011 of 564.8, current prices for these columns were calculated.

The following values for costing a double pipe heat exchanger were used:

- $K_1 = 4.4646$
- $K_2 = -0.5277$
- $K_3 = 0.3955$

The following values for costing a kettle reboiler were used:

- $K_1 = 3.3444$
- $K_2 = 0.2745$
- $K_3 = -0.0472$

The following  $A$  values were calculated and based on the minimum and maximum values suggested by the CAPCOST program, prices were adjusted:

Column	Condenser/Reboiler	$A \text{ (m}^2\text{) calculated}$	$A \text{ (m}^2\text{) used}$	$C_p^0 \text{ in 2001 (\$)}$	$C_p^0 \text{ in 2011 (\$)}$
Column 1	Condenser	0.00035	1	2,210	3,144
Column 2	Condenser	0.000038	1	2,210	3,144
Column 3	Condenser	0.00073	1	2,210	3,144
Column 4	Condenser	0.00011	1	2,210	3,144
Column 1	Reboiler	0.0048	10	3,730	5,306
Column 2	Reboiler	0.000245	10	3,730	5,306
Column 3	Reboiler	0.0018	10	3,730	5,306
Column 4	Reboiler	0.000039	10	3,730	5,306

Table 8: **Distillation column costing using CAPCOST**



### Appendix IX - Utilities Costing (Based on 10-Year Plant Life)

Utilities used for the condensers and reboilers associated with the distillation columns were considered. Pure liquid nitrogen, cooling/pure water, and three different types of steams were used based on the desired temperature changes in the streams.

An example of how sizing and costing of heat exchangers and utilities is shown below using the condenser of Column 1. The vapor going into the condenser is at 382 K and the stream leaving the condenser is at 275 K. The heat duty is known from Pro/II to be 273 kJ/hr. Because a utility is needed at a temperature lower than 275 K, cooling water at 305 K, although cheaper was not sufficient. Thus, liquid nitrogen, at 77 K was chosen. The boiling point of nitrogen at this column's top tray pressure is approximately 83 K (DIPPR) and it was assumed that nitrogen at 77 K is close enough to this point that the heat of vaporization can be used to determine the mass flow rate of the utility needed. Due to this assumption, the temperature change of the nitrogen was taken to be 82.62 K to 83.62 K.

$$Q = \dot{m}H_{vap} \rightarrow \dot{m} = \frac{Q}{H_{vap}} \quad (27)$$

$$\dot{m} = \frac{272.7 \text{ kJ/hr}}{5346 \text{ kJ/kmol}} = 0.05 \text{ kmol/hr of pure liquid nitrogen needed} \quad (28)$$

Costing information for pure liquid nitrogen was given to be \$0.10/L at 77 K. I am not sure if a heat exchanger would be necessary to get the nitrogen up to its boiling point but the temperature difference is small between 77 K and 83 K so I will consider it negligible. Several unit conversions were done to determine the volume of liquid nitrogen per hour is needed. Costing was done for a plant that operates 365 days/year. Most likely, this will not happen due to maintenance work and other unexpected events so again, this will be an overestimation of utility costs.

$$\frac{0.05 \text{ kmol/hr}}{27.83 \text{ kmol/m}^3} = 0.0017 \text{ m}^3/\text{hr} \quad (29)$$

$$0.0017 \text{ m}^3/\text{hr} \times 1000 \text{ L/m}^3 = 1.7 \text{ L/hr} \quad (30)$$

$$1.7 \text{ L/hr} \times \$0.10/\text{L} = \$0.17/\text{hr} \quad (31)$$

$$\$0.17/\text{hr} \times 24\text{hr/day} \times 365\text{days/year} = \$1,522/\text{year} \quad (32)$$

(Note: Numbers may be slightly off because of round-off error. Calculations were done using more significant figures and rounded off at the end)

For utilities used that were not near their boiling points such as for cooling water or where it was irrelevant to use the heat of vaporization such as in the case of steam in the reboilers, the specific heats of these utilities were used to determine mass flow rate needed for these utilities and size of the heat exchangers:

$$Q = \dot{m}c_p\Delta T \rightarrow \dot{m} = \frac{Q}{c_p\Delta T} \quad (33)$$

Using similar methods as above (different unit conversions based on costing information units), the price for each utility was determined:

The cost for each utility used is given below:

Column	Condenser/Reboiler	Utility Used	Mass Flow Rate (kmol/hr)	Price (\$/year)
Column 1	Condenser	Liquid nitrogen	0.048	1522
Column 2	Condenser	Liquid nitrogen	0.0036	114
Column 3	Condenser	Cooling water	0.013	0.04
Column 4	Condenser	Liquid nitrogen	0.0059	186
Column 1	Reboiler	125# steam	0.23	363
Column 2	Reboiler	20# steam	0.031	35
Column 3	Reboiler	125# steam	0.056	71
Column 4	Reboiler	20# steam	0.0076	8

Table 9: **Utilities costing**

Utility	Cost
Pure liquid nitrogen (77K)	\$0.10/L
Cooling pure water (90F)	\$0.08/1000 gallons
600# steam (490F, HP)	\$10/metric ton
125# steam (353F, MP)	\$8/metric ton
20# steam (260F, LP)	\$7/metric ton

Table 10: **Utilities costing information**

**Appendix XI - Costing Summary**

Equipment/Utilities	Price (\$)
Column Shells	11700
Column Trays	17100
Condensers	$(3,144 \times 4) = 12600$
Reboilers	$(5306 \times 4) = 21200$
Membrane	$(22,500 \times 10) = 225,000$
Liquid nitrogen	$(1522+114+186) \times 10 = 18200$
Cooling water	$(0.04 \times 10) = \$0.40$
125# steam	$(363+71 \times 10) = \$4340$
60# steam	$(35+8 \times 10) = 430$
Total	\$310570

Table 11: **Costing summary (capital costs and utilities cost for 10-year plant life)**

Note: It was estimated that the membrane is replaced once a year.

**Appendix XII - Detailed Tables of All Calculations**

See attached pages.

## MEMO

**To:** Benjamin Davis, Project Manager, C Squared Consulting Associates, 41 Cooper Square, NY, NY 10003

**From:** Student 2, Design Engineer, C Squared Consulting Associates, 41 Cooper Square, NY, NY 10003

**Subject:** Revised Proposal for Separation of a Four Component Mixture

**Date:** Tuesday, January 16, 2012

This is a memo regarding a revised proposal for a separation plant to separate a 1000 kg mixture of ethylbenzene (90%), ethanol (8%), ammonia (1%) and hydrogen sulfide (1%). Like the previous evaluation, thermodynamic data was based on the Peng-Robinson model (including entropy and enthalpy values for minimum work calculations), and separation units were sized and costed. Sizing was done using Pro/II and confirmed by graphical methods. Costing was based on Analysis, Synthesis, and Design of Chemical Processes, by Turton *et al.*, 2nd edition.

This revised design is comprised of only four distillation columns. Although this design costs more, I am recommending it because it is possible for these columns to be built. They are not unreasonably skinny like the previous PFD. It separates the mixture to four streams with at least 99% purity by mole while expending less than ten times the minimum work required to perform such a separation. The sizes of these columns are much bigger than the initial proposal. Diameters range from 8 to 33 ft and heights range from 27 to 53 ft. Although these columns can be built, this plant would be abnormally large. Based on Turton *et al.*, the linear velocity was assumed to be 2 ft/sec. Consequently, the cost of the column shells and trays are higher than the previous proposal, totaling about \$1.7 million. Reboilers and condensers were sized to have areas ranging from  $3 \times 10^{-1}$  to  $1.8 \text{ ft}^2$  and costing was based on prices for kettle reboilers and double pipe condensers. Costing for these heat exchangers were overestimated because costing information was only valid for equipment larger than those specified in this PFD. Total costs for heat exchangers came to \$33,000. This is comparable to the heat exchangers costed for the previous PFD.

Taking into account the utilities that are needed for the condensers and reboilers, capital and annual costs for that time period total to about \$31 million. This is much more expensive than the initial proposal. Again, these sizes are large for separation units and because of this, I am requesting more time for a final proposal of this separation plant design. During this time, I will discuss with my colleagues possible explanations as to why these designs are not like previous separation plants designed in terms of size. Also, I will calculate the linear velocity of the vapor more rigorously instead of using Turton *et al.*'s heuristics. Another reason why some of these columns have such large diameters is because the number of trays was optimized for each column but the reflux ratio was not fully optimized for the desired specifications.

See appendices for a PFD of this design, mass balances, confirmation that at least 90% of mass is recovered, confirmation of thermodynamic feasibility and Pro/II calculations, and more details. Let me know if you have any questions or suggestions, and I will keep you posted on future work.

## Appendices

### Appendix I - Process Flow Diagram

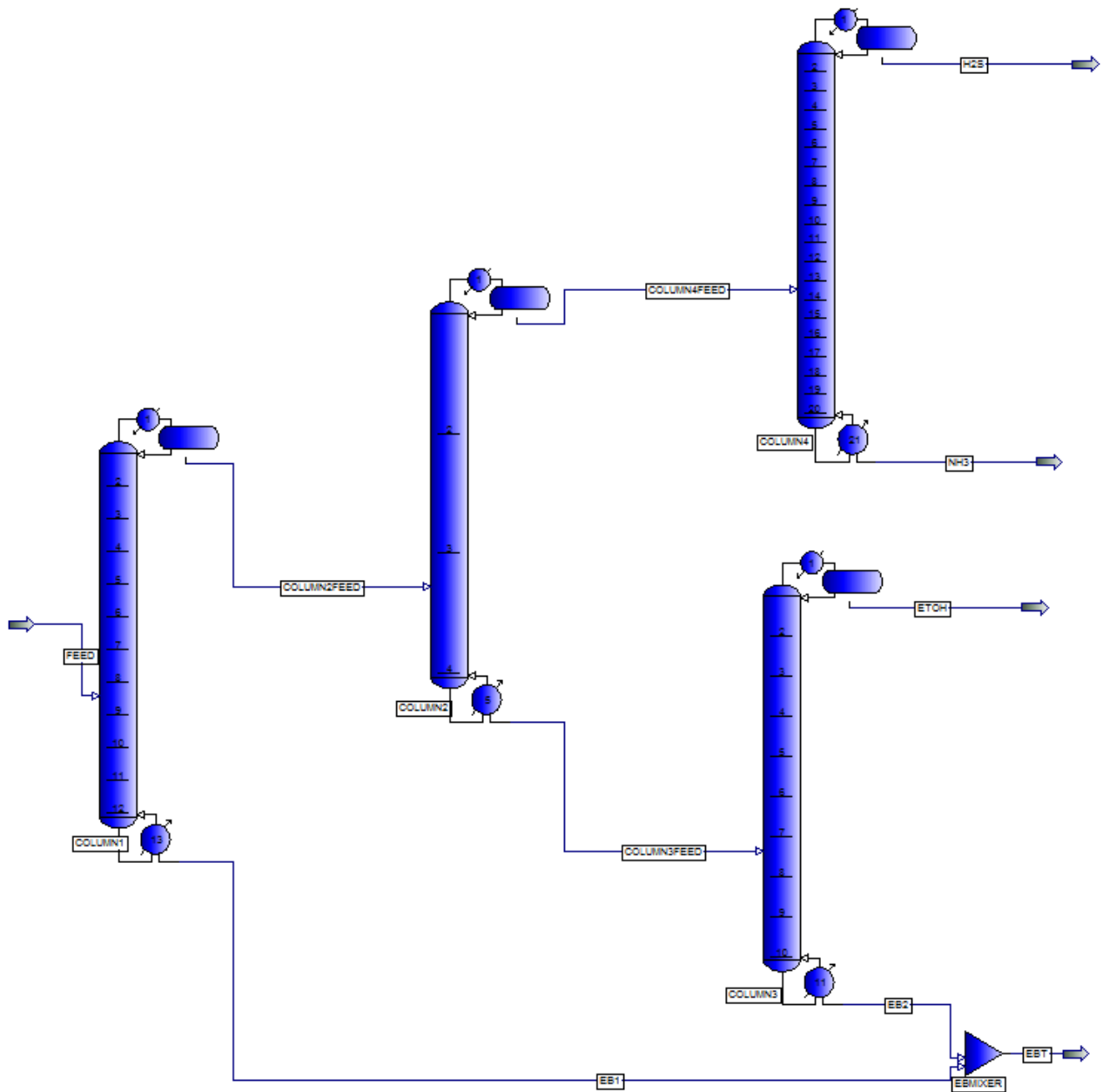


Figure 2: **Process flow diagram of revised proposal for separation of ethylbenzene (90%), ethanol (8%), ammonia (1%), & hydrogen sulfide (1%).**

**Appendix I (cont'd)**

In order to understand qualitatively and quantitatively how the mixture is being separated in the PFD, note that ethylbenzene is abbreviated as EB, ethanol as ETOH, ammonia as NH<sub>3</sub>, and hydrogen sulfide as H<sub>2</sub>S. See tables below for more details.

PFD Label Name	Description of Equipment/Feed
FEED	Contains EB (90%), ETOH (8%), NH <sub>3</sub> (1%), and H <sub>2</sub> S (1%), 1000 kg/hr
COLUMN1	Separates out EB, Light Key (LK): ETOH, Heavy Key (HK): EB
EB1	Stream of 99.9% EB by mole; To be mixed with EB2 to give EB product stream
COLUMN2FEED	Contains more than half ETOH
COLUMN2	Separates ETOH from NH <sub>3</sub> and H <sub>2</sub> S (LK: NH <sub>3</sub> , HK: ETOH)
COLUMN3FEED	Contains mostly ETOH
COLUMN3	Separates ETOH from EB (LK: ETOH, HK: EB)
EB2	Stream of 99% EB; To be mixed with EB1 to give EB product stream
EBMIXER	Mixes EB1 & EB2 to give EB product stream
EBT	EB product stream, 99.09% EB by mole, 8.47 kmol/hr
ETOH	Ethanol product stream, 98.8% ETOH by mole, 1.746 kmol/hr
COLUMN4FEED	Contains mostly NH <sub>3</sub> (66%) and H <sub>2</sub> S(33%)
COLUMN4	Separates NH <sub>3</sub> and H <sub>2</sub> S
NH3	NH <sub>3</sub> product stream, 99.7% NH <sub>3</sub> by mole, 0.586 kmol/hr
H2S	Hydrogen sulfide product stream, 99.7% H <sub>2</sub> S by mole, 0.586 kmol/hr

Table 12: **Description of PFD labels.**

Component/Parameter	FEED	Stream											
		COLUMN2FEED		EB1	COLUMN4FEED		COLUMN3FEED		ETOH	EB2	H2S	NH3	EBENZENET
	Mixed	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Liquid	Mixed
Temperature (F)	170.3	35.6	338.9	-26.1	222.8	213.1	344.9	-51.3	4.9	338.6			
Pressure (psia)	29.4	29.0	34.0	29.0	34.0	34.0	39.0	29.0	34.0	34			
Ethylbenzene	0.764	0.156	0.999	0	0.218	0.011	0.986	0	0	0.999			
Ammonia	0.053	0.190	0	0.666	0.001	0.001	0	0.003	0.997	0			
Hydrogen sulfide	0.026	0.095	0	0.333	0	0	0	0.997	0.002	0			
Ethanol	0.157	0.559	0.001	0.001	0.781	0.968	0.014	0	0.001	0.001			

Table 13: Composition and molar flow rates of all streams.



**Appendix II - Mass Recovered**

To confirm that no more than 90% of the original feed's mass was lost to waste or burned for heat, the mass recovered was determined by summing the mass flow rates of the product streams and comparing it to the mass flow rate of the feed.

Product Stream	Molar Flow Rate (kmol/hr)
EB	8.5
ETOH	1.7
NH3	0.6
H2S	0.3
Total	11.1

Table 14: **Molar flow rates of outlet/product streams.**

The inlet feed's molar flow rate was 11.1 kmol/hr. The percent of mass recovered:

$$\frac{\text{Mass Flow Rate In}}{\text{Mass Flow Rate Out}} = \frac{11.1}{11.1} \times 100\% = 100\% \quad (34)$$

This confirms that no mass was lost due to waste streams or burned for heat. This fulfills the requirement that no more than 90% of the mass should be wasted.

### Appendix III - Calculation and Comparison to Minimum Work Required

The minimum work of separation is defined as (Separation Process Principles, by Seader *et al.*:

$$W_{min} = \Sigma_{out} nb - \Sigma_{in} nb \quad (35)$$

where

$$b = h - T_0 s \quad (36)$$

and  $T_0$  = ambient temperature

There was one stream into the system (FEED) and four streams coming out of the system (EB, ETOH, NH<sub>3</sub>, H<sub>2</sub>S). For each stream,  $nb$  was calculated:

$$nb = \dot{m} \times (h - T_0 s) \quad (37)$$

where  $\dot{m}$  = mass flow rate (kg/hr),  $h$  = specific enthalpy (BTU/kg),  $T_0$  = ambient temperature (F),  $s$  = specific entropy (BTU/kgF)

For FEED:

$$1000 \text{ kg/hr}(150.03 \text{ BTU/kg} - (300 \text{ F} * 2.54 \text{ BTU/kgF})) = -610993 \text{ BTU/hr} \quad (38)$$

For EBT:

$$898.18 \text{ kg/hr}(310.41 \text{ BTU/kg} - (300 \text{ F} * 2.71 \text{ BTU/kgF})) = -450354 \text{ BTU/hr} \quad (39)$$

For ETOH:

$$81.48 \text{ kg/hr}(253.4 \text{ BTU/kg} - (300 \text{ F} * 2.73 \text{ BTU/kgF})) = -46176 \text{ BTU/hr} \quad (40)$$

For NH<sub>3</sub>:

$$10.02 \text{ kg/hr}(-47.88 \text{ BTU/kg} - (300 \text{ F} * 3.39 \text{ BTU/kgF})) = -10673 \text{ BTU/hr} \quad (41)$$

For H<sub>2</sub>S:

$$9.97 \text{ kg/hr}(-79.4 \text{ BTU/kg} - (300 \text{ F} * 1.79 \text{ BTU/kgF})) = -6150 \text{ BTU/hr} \quad (42)$$

Calculating  $W_{min}$ ,

$$W_{min} = (-450354 + -46176 + -10673 + -6150) - (-610993) = 97641 \text{ BTU/hr} \quad (43)$$

The maximum  $W$  allowed is ten times  $W_{min}$  which is 976410 BTU/hr.

To determine the work used in this PFD, the heat duties of all of the reboilers and condensers were considered: Heat duties of reboilers were contributed to the work used and those of the condensers released work that could be used elsewhere.

**Appendix III - Calculation and Comparison to Minimum Work Required**

Equipment	Heat Duty (BTU/hr)
Column 1, Condenser	-258300
Column 1, Reboiler	371800
Column 2, Condenser	-105800
Column 2, Reboiler	136800
Column 3, Condenser	-86900
Column 3, Reboiler	90300
Column 4, Condenser	-19800
Column 4, Reboiler	20100

Table 15: **Work used/released by column condensers and reboilers.**

Based on the values in Table 15, work used in this PFD was calculated to be 148200 BTU/hr, which is well under the maximum allowable work to be used for the separation.

### Appendix IV - Number of Trays of Column from Pro/II & Graphical Confirmation of Distillation Column Sizing for Columns 1-4

Column	Number of Trays
Column 1	13
Column 2	5
Column 3	11
Column 4	21

Table 16: Number of trays in distillation columns from Pro/II.

For confirmation, see appendices from initial proposal and attached page for these calculations done graphically via McCabe-Thiele Method. The number of trays determined graphically were of the same magnitude as those found via Pro/II (above). The McCabe-Thiele Method is outlined below:

1. Generate binary vapor liquid equilibrium data and  $x = y$  line using Pro/II. Specify the light key as the "first component"
2. Determine the concentration of the light key in the feed ( $z_f$ ), the concentration of the light key in the distillate ( $x_D$ ), and the concentration of the light key in the bottoms ( $x_B$ ).
3. Determine  $q$  based on the conditions of the feed.
4. Determine  $q$ -line equation based on its equation:

$$y = \left(\frac{q}{q-1}\right)x - \frac{z_F}{q-1} \quad (44)$$

5. Because all feeds were assumed to be liquid,  $q = 1$  and  $q$ -lines were vertical and passed through  $z_F$  on the  $x$ -axis.
6. The minimum L/V lines were drawn - the rectifying section passed through the  $x=y$  line at  $x = 0.99$  and where the  $q$ -line intersects the equilibrium curve, and the stripping section passed through where the  $q$ -line intersects the equilibrium curve and the  $x=y$  lines at  $x = 0.01$ .
7. The minimum number of trays was determined by drawing steps between the  $x=y$  line and the equilibrium curve.
8. The slope of the L/V minimum line, rectifying section, was found and set to  $\frac{R_{min}}{R_{min}+1}$ .  $R_{min}$  was calculated.
9. The following relationship from Turton et al. heuristics was used to determine  $R$ ,  $R = 1.5R_{min}$ .
10. This value of  $R$  was used to determine the slope of the actual L/V line, rectifying section.

11. The actual L/V line was plotted and steps were drawn between this line and the equilibrium curve to determine the actual number of trays.

Please note the following things about the graphs:

- One McCabe-Thiele plot was done for Columns 1, 2, 3 for initial and revised designs because similar if not the same conditions (pressure of feed, and compositions of the feed, distillate, and bottoms) occurred
- A ratio of 1.5 for  $R/R_{min}$  was used based on heuristics from Turton *et al.*. This differs from the  $R$  used in Pro/II calculations. This may contribute to discrepancies between the actual trays numbers calculated by Pro/II and graphically.
- The blue line in each plot is the  $45^\circ$  line, which represents the reflux ratio when there is infinite reflux.
- The green line in each plot represents the equilibrium data for the binary mixture.
- The composition of the light key  $z_f$  used in the plot was adjusted when assuming a pseudo-binary mixture using the following normalization:

$$z_f = \frac{\text{Mole fraction of Light Key}}{\text{Mole fraction of Light Key} + \text{Mole fraction of Heavy Key}} \quad (45)$$

- The mole fractions of the light key in the distillate and bottoms ( $x_D$  and  $x_B$  respectively) was calculated from Pro/II results and if they were greater than 0.99 or less than 0.01, respectively, values were just taken to be 0.99 or 0.01, respectively because it is difficult to graph values greater than 0.99 or less than 0.01.
- It was assumed that all feeds were at its bubble point so all the feed was a liquid. This led  $q$  to equal 1 and the  $q$ -line to always be a vertical line that passed through  $z_f$ , the composition of the light key in the feed.
- The "count" of the minimum number of trays is "inside" the step on the graph and the "count" of the actual number of trays is "outside" the step on the graph.

## Appendix V - Diameter Sizing for Columns 1-4

Below is a sample calculation for how the height and diameter was sized for Column 1. See attached page for heights and diameters of Columns 2 - 4.

For column 1:

### Height of a Distillation Column

Based on heuristics from Turton *et al.* (Chapter 9, Table 9.13 and 9.14), tray spacings were assumed to be 20 inches. Heuristics also give heights for top spacing for vapor disengagement and bottom spacing for liquid level and reboiler return based on a 3 ft in diameter column. Based on a 3 ft diameter, top spacing was 4 ft and bottom spacing was 6 ft. Space at the top and bottom were calculated in proportion to the diameter of the designed columns but a maximum of 20 ft for both the top and bottom spacings were added. For column 1, the top spacing and the bottom spacing were calculated to be greater than 20 ft. so 20 ft. was used as the combined height of the top and bottom spacings.

To determine the height of the column:

$$(\text{Number of Trays} - 1) \times (\text{Tray Spacing}) + \text{Top Spacing} + \text{Bottom Spacing} = \text{Height} \quad (46)$$

$$(13 - 1) \times (20 \text{ in.}) + 10 \text{ ft} + 10 \text{ ft} = 40 \text{ ft} \quad (47)$$

**Diameter of a Distillation Column** The maximum vapor flow rate was determined to be 5973000 ft<sup>3</sup>/hr from the Pro/II report. Based on heuristics from Turton *et al.*, the linear velocity of the vapor was assumed to be 2 ft/sec.

To determine the area of the tray needed for this vapor flow rate to pass at that specified velocity,

$$\frac{\text{Vapor flow rate}}{\text{Linear velocity}} = \text{Area} \quad (48)$$

$$\frac{5973000 \text{ ft}^3/\text{hr}}{7200 \text{ ft/hr}} = 830 \text{ ft}^2 \quad (49)$$

$$\text{Diameter} = 2 \times \left( \sqrt{\frac{\text{Area}}{\pi}} \right) \quad (50)$$

$$\text{Diameter} = 2 \left( \sqrt{830/\pi} \right) = 32.5 \text{ ft} \quad (51)$$

Using these methods of calculation for heights and diameters of columns:

Column	Height (ft)	Diameter (ft)
Column 1	40	32.5
Column 2	26.7	18.3
Column 3	36.7	14.6
Column 4	53.3	8.2

Table 17: Distillation columns sizing based on Pro/II results and heuristics.

## Appendix VI - Capital Costing (Columns and Membrane)

Using cost equations for the CAPCOST Program as specified in Turton *et al.*, sizing parameters such as area and volume were used to determine costs of the shell and trays of the column. Purchased equipment costs were determined by:

$$\log(C_p^0) = K_1 + K_2 \log(A) + K_3 [\log(A)]^2 \quad (52)$$

where  $A$  is the sizing parameter,  $K_1$ ,  $K_2$ , and  $K_3$  are constants,  $C_p^0$  is the purchased equipment costs for 2001. Using the CEPCI value for 2001 of 397 and the CEPCI value for 2011 of 564.8, current prices for these columns were calculated.

CAPCOST cost equations were fitted to columns of a specified size. If a designed column was smaller than the specified size, the minimum  $A$  value was used and thus, the cost was overestimated. If a designed column was larger than the specified size, the maximum  $A$  value was used and the price was estimated assuming a linear relationship between  $A$  and price.

For column 1:

- Volume ( $\text{m}^3$ ) = 940
- Area ( $\text{m}^2$ ) = 77
- For shell costing,  $A = 520$
- For shell costing,  $K_1 = 3.94974$ ,  $K_2 = 0.4485$ ,  $K_3 = 0.1074$
- For tray costing,  $A = 12$
- For tray costing,  $K_1 = 2.9949$ ,  $K_2 = 0.4465$ ,  $K_3 = 0.3961$

Using the above values and Equation 17, costs for year 2001 were calculated to be:

- Cost of Shell in 2001: \$673,000
- Cost of Trays in 2001: \$232,000

Using 2011 CEPCI value of 564.8 (from *Chemical Engineering, April 2011*) and 2001 CEPCI value of 397,

- Cost of Shell in 2011: \$958,000
- Cost of Trays in 2011: \$1,189,133

Using the above method, the following costs were calculated for Columns 2-4:

Note that because these columns were on the large side, the maximum  $A$  specified in the heuristics were used for Columns 2-4 and a linear relationship between price and sizing after the maximum  $A$  value was assumed.

Column	Shell Cost (\$)	Tray Cost (\$)
Column 1	958,000	1,190,000
Column 2	177,000	211,000
Column 3	156,000	173,000
Column 4	78,000	82,000
Total	1,370,000	1,660,000

Table 18: **Distillation column costing using CAPCOST**



## Appendix VIII - Heat Exchanger Sizing & Costing

The heat duty ( $Q$ ) from Pro/II was used to determine the area of the heat exchanger needed:

$$Q = UA\Delta T_{lm} \rightarrow A = \frac{Q}{U\Delta T_{lm}} \quad (53)$$

Based on heuristics from Turton *et al.*,  $U$  was taken to be 850 W/m<sup>2</sup> and 1150 W/m<sup>2</sup> for condensers and reboilers, respectively.

For the condenser for Column 1,

$$\Delta T_{lm} = \frac{\Delta T_1 - \Delta T_2}{\ln \frac{T_1}{T_2}} \quad (54)$$

- $T_{stream,in} = 381.6\text{K}$
- $T_{stream,out} = 275.2\text{K}$
- $T_{utility,in} = 82.62\text{K}$
- $T_{utility,out} = 83.62\text{K}$
- $\Delta T_1 = T_{stream,in} - T_{utility,out} = 381.6 - (83.62) = 97.98 \text{ K}$
- $\Delta T_2 = T_{stream,out} - T_{utility,in} = 275.2 - (82.62) = 192.6 \text{ K}$
- $\rightarrow \Delta T_{lm} = 241.46$

$$A = \frac{75694 \text{ J/sec}}{(850 \text{ W/m}^2)(241.46)} = 0.37 \text{ m}^2 \quad (55)$$

Based on the CAPCOST program delineated in Turton *et al.*, the cost of heat exchangers were determined. Double pipe heat exchangers were chosen for condensers because the smallest heat exchangers do come in that type. Kettle reboilers' cost information was used for this project because kettle reboilers were chosen in the Pro/II design. The CAPCOST equation was used:

$$\log(C_p^0) = K_1 + K_2 \log(A) + K_3 [\log(A)]^2 \quad (56)$$

where  $A$  is the sizing parameter,  $K_1$ ,  $K_2$ , and  $K_3$  are constants,  $C_p^0$  is the purchased equipment costs for 2001. Again, using the CEPCI value for 2001 of 397 and the CEPCI value for 2011 of 564.8, current prices for these columns were calculated.

The following values for costing a double pipe heat exchanger were used:

- $K_1 = 4.4646$
- $K_2 = -0.5277$
- $K_3 = 0.3955$

The following values for costing a kettle reboiler were used:

- $K_1 = 3.3444$
- $K_2 = 0.2745$
- $K_3 = -0.0472$

The following  $A$  values were calculated and based on the minimum and maximum values suggested by the CAPCOST program, prices were adjusted:

Column	Condenser/Reboiler	$A \text{ (m}^2\text{) calculated}$	$A \text{ (m}^2\text{) used}$	$C_p^0 \text{ in 2001 (\$)}$	$C_p^0 \text{ in 2011 (\$)}$
Column 1	Condenser	0.00037	1	2,210	3,144
Column 2	Condenser	0.22	1	2,210	3,144
Column 3	Condenser	0.77	1	2,210	3,144
Column 4	Condenser	0.05	1	2,210	3,144
Column 1	Reboiler	1.66	10	3,730	5,306
Column 2	Reboiler	0.68	10	3,730	5,306
Column 3	Reboiler	1.7	10	3,730	5,306
Column 4	Reboiler	0.03	10	3,730	5,306

Table 19: **Heat exchanger costing using CAPCOST**

### Appendix IX - Utilities Costing (Based on 10-Year Plant Life)

Utilities used for the condensers and reboilers associated with the distillation columns were considered. Pure liquid nitrogen, cooling/pure water, and three different types of steams were used based on the desired temperature changes in the streams.

An example of how sizing and costing of heat exchangers and utilities is shown below using the condenser of Column 1. The vapor going into the condenser is at 382 K and the stream leaving the condenser is at 275 K. The heat duty is known from Pro/II to be 273 kJ/hr. Because a utility is needed at a temperature lower than 275 K, cooling water at 305 K, although cheaper was not sufficient. Thus, liquid nitrogen, at 77 K was chosen. The boiling point of nitrogen at this column's top tray pressure is approximately 83 K (DIPPR) and it was assumed that nitrogen at 77 K is close enough to this point that the heat of vaporization can be used to determine the mass flow rate of the utility needed. Due to this assumption, the temperature change of the nitrogen was taken to be 82.62 K to 83.62 K.

$$Q = \dot{m}H_{vap} \rightarrow \dot{m} = \frac{Q}{H_{vap}} \quad (57)$$

$$\dot{m} = \frac{272500 \text{ kJ/hr}}{5346 \text{ kJ/kmol}} = 51 \text{ kmol/hr of pure liquid nitrogen needed} \quad (58)$$

Costing information for pure liquid nitrogen was given to be \$0.10/L at 77 K. I am not sure if a heat exchanger would be necessary to get the nitrogen up to its boiling point but the temperature difference is small between 77 K and 83 K so I will consider it negligible. Several unit conversions were done to determine the volume of liquid nitrogen per hour is needed. Costing was done for a plant that operates 365 days/year. Most likely, this will not happen due to maintenance work and other unexpected events so again, this will be an overestimation of utility costs.

$$\frac{51 \text{ kmol/hr}}{27.83 \text{ kmol/m}^3} = 1.83 \text{ m}^3/\text{hr} \quad (59)$$

$$1.83 \text{ m}^3/\text{hr} \times 1000 \text{ L/m}^3 = 1832 \text{ L/hr} \quad (60)$$

$$1832 \text{ L/hr} \times \$0.10/\text{L} = \$183/\text{hr} \quad (61)$$

$$\$183/\text{hr} \times 24\text{hr/day} \times 365\text{days/year} = \$1.6\text{million/year} \quad (62)$$

(Note: Numbers may be slightly off because of round-off error. Calculations were done using more significant figures and rounded off at the end)

For utilities used that were not near their boiling points such as for cooling water or where it was irrelevant to use the heat of vaporization such as in the case of steam in the reboilers, the specific heats of these utilities were used to determine mass flow rate needed for these utilities and size of the heat exchangers:

$$Q = \dot{m}c_p\Delta T \rightarrow \dot{m} = \frac{Q}{c_p\Delta T} \quad (63)$$

Using similar methods as above (different unit conversions based on costing information units), the price for each utility was determined:

The cost for each utility used is given below:

Column	Condenser/Reboiler	Utility Used	Mass Flow Rate (kmol/hr)	Price (\$/year)
Column 1	Condenser	Liquid nitrogen	51	1,600,000
Column 2	Condenser	Liquid nitrogen	21	660,000
Column 3	Condenser	Cooling water	14	47
Column 4	Condenser	Liquid nitrogen	4	120,000
Column 1	Reboiler	125# steam	235	370,000
Column 2	Reboiler	20# steam	82	90,000
Column 3	Reboiler	125# steam	60	75,000
Column 4	Reboiler	20# steam	13	15,000

Table 20: **Utilities costing**

Utility	Cost
Pure liquid nitrogen (77K)	\$0.10/L
Cooling pure water (90F)	\$0.08/1000 gallons
600# steam (490F, HP)	\$10/metric ton
125# steam (353F, MP)	\$8/metric ton
20# steam (260F, LP)	\$7/metric ton

Table 21: **Utilities costing information**

**Appendix XI - Costing Summary**

Equipment/Utilties	Price (\$)
Column Shells	1.4 million
Column Trays	290,000
Condensers	$(3,144 \times 4) = 12600$
Reboilers	$(5306 \times 4) = 21200$
Membrane	$(22,500 \times 10) = 225,000$
Utilities (10-year plant life)	29 million
Total	\$31 million

**Table 22: Costing summary (capital costs and utilities cost for 10-year plant life)**

**Appendix XII - Detailed Tables of All Calculations**

See attached pages.